

Propyl carbamate
627-12-3 | DTXSID7060833

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.25 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.79e-01

Confidence level: 6.88e-01

Nearest Neighbors from the Training Set

Image not found

Propyl carbamate

Measured: 7.41e-01

Predicted: 1.25

Image not found

Acrylamide

Measured: 9.00

Predicted: 9.79

Image not found

2-Fluoroacetamide

Measured: 13.0

Predicted: 12.6

Image not found

Acetamide

Measured: 38.1

Predicted: 19.0